From Cooper-pairs to resonating bipolarons

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I. INTRODUCTION

By far the most decisive experimental results which led the way in acquiring a theoretical understanding of superconductivity was (i) the Meissner effect and (ii) the isotope shift in the critical temperature T_c.

Fritz and Heinz London early on recognized[1] that the Maxwell equations had to be supplemented by a relation between the magnetic field applied to a superconductor and the thereby induced macroscopic circulating currents, in order to account for the expulsion of such an externally applied magnetic field from the inside of the superconducting sample. The shielding supercurrents necessarily being a macrosocopic feature, Fritz London conjectured this to be a manifestation of the Bose Einstein condensation, according to which the charge carriers making up such supercurrents are condensed into a single quantum state—now generally refered to as macroscopic coherent quantum state. Invoking the Heisenberg uncertainty principle, the charge carriers making up such spatially homogeneous supercurrents moving on huge orbitals, suggested that any order defining such a superconducting state must be an order in momentum rather than real space of the charge carriers. Since it could be expected that the electrons participating in the supercurrents came from only a very small region in **k**-space around the Fermi surface, this insight served as a hint of vital importance in the construction of the ultimate solution for the superconducting ground state wave function[2].

The other such vital hint helping to solve the ridle of the superconductivity phenomenon came from the theoretical work by H. Fröhlich[3,4], who showed that, inspite of the heavy mass of the ions and the repulsive Coulomb interaction between the electrons, two electrons near the Fermi surface will interact attractively with each other. He suggested that the difference in energy beween the superconducting and the normal state of a metal could result from such electron lattice interaction. The experiments[5] on the isotope shift of the critical temperature of superconductors, carried out at the same time and totally indepedent on any knowledge of these theoretical results, strongly supported this suggestion.

Given the insight coming from the Meissner effect and the isotope shift in T_c, the problem then was to put that knowledge on a firm theoretical ground. This was done in the seminal work by Bardeen, Cooper and Schrieffer[2]. Inspite of the success in explaining the isotope shift of T_c as arising from an effective lattice modulated electron-electron interaction[3,4], this initial work was in an order of magnitude conflict with the experimentally observed energy difference between the superconducting and the normal state. This difficulty was overcome in a study considering the interaction of just two electrons above an immobile Fermi sea[6] and clearly indicated the instability of the Fermi sea as a result of the electron-lattice interaction. The final remaining task then was to repeat this study for the ensemble of electrons in the Fermi sea. This was achieved in what is now known as the BCS wavefunction[2], constructed in such a way that the electrons optimally exploit the electron-lattice coupling in their scattering processes, allbeit in full respect of the Pauli principle. The BCS theory relates the appearence of the superconducting state to the appearence of Cooper-pair formation. This is manifest in the developement of a finite amplitude of the order parameter, which shows up in form of a gap in the single particle electron specrum. The role of the phase of the order parameter in this superconducting BCS ground state, which is a prerequisit of any coherent macroscopic quantum state and necessary to assuring the Meissner effect[7], is hidden in this early BCS formulation and which, in a more transparent way, was subsequently provided by P. W. Anderson[8].

The BCS theory for electron-lattice induced superconductivty applies to systems with weak electron lattice interaction, implying a small energy gap over Fermi energy ratio $\Delta(0)/\varepsilon_F \ll 1$ and the adiabatic regime $k_B\theta_D/\varepsilon_F \ll 1$, with θ_D denoting the Debye frequency. The question which has occupied the superconductivity community for some time is to establish what happens to such a BCS superconductor if those conditions are no longer satisfied. Intuitively one could expect[9] that upon increasing the electron-lattice interaction would ultimately lead to a local polaron type instability of the lattice structure surrounding the charge carriers and hence give rise to localization. On the other hand, provided one is in an anti-adiabatic regime (with a characteristic local lattice vibrational mode energy much bigger than the bare electron hopping integral), one obtains a superfluid phase of local electron-pairs, the socalled Bipolaronic Superconductivity[10]. The cross-over between the BCS regime either to a superfluid state of tightly bound electron pairs or to their localization is presently a field of great interest. In the following sections we shall review the issues involved in such a physics.

II. FROM AMPLITUDE TO PHASE FLUCTUATION CONTROLLED SUPERCONDUCTIVITY

Let us consider a quite general electron-lattice coupling Hamiltonian

$$\begin{aligned} H &= H_{\rm el} + H_{\rm ph} + H_{\rm el,ph} \\ &= \sum_{\mathbf{k}\sigma} (\varepsilon_{\mathbf{k}} - \mu) c^+_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} + \sum_{\mathbf{q}} \omega_{\mathbf{q}} \left(a^+_{\mathbf{q}} a_{\mathbf{q}} + \frac{1}{2} \right) \\ &+ \sum_{\mathbf{qk}\sigma} V_{\mathbf{q}} c^+_{\mathbf{k+q}\sigma} c_{\mathbf{k}\sigma} (a_{\mathbf{q}} + a^+_{-\mathbf{q}}) \end{aligned} \tag{1}$$

which permits us to describe the essential features of BCS as well as of Bipolaronic Superconductivity in the simplest possible way. $c^+_{\mathbf{k}\sigma}, c_{\mathbf{k}\sigma}$ denote bare electron creation and annihilation operators for Bloch states characterized by momenta $\mathbf{k}$ and spin σ and having a bare electron spectrum given by $\varepsilon_{\mathbf{k}}$. $a^+_{\mathbf{q}}, a_{\mathbf{q}}$ denote creation, respectively annihilation operators for phonons with wave vectors $\mathbf{q}$ and having bare phonon frequencies $\omega_{\mathbf{q}}$. Finally, $V_{\mathbf{q}}$ denotes an effective electron-phonon coupling, the effect of which is twofold: (i) to "delocalize" the Bloch states, i.e., the electron momentum being no longer a conserved quantity speads the resulting excitations around the wavevectors which characterize the system in the absence of the electron-phonon coupling, (ii) to induce lattice deformations in the neighborhood of the momentary positions of the electrons on the lattice. Effective Hamiltonians which capture these features can be constructed by use of unitary transformations $\tilde{H} = e^{-S} H e^{S}$ with

$$S = \sum_{\mathbf{i}\,\mathbf{j}\,l\,\sigma} c^+_{\mathbf{i}\sigma} c_{\mathbf{j}\sigma} (\pi_{(j-i,\, l-i)} P_{\mathbf{l}} + \chi_{(j-i,\, l-i)} X_{\mathbf{l}}) \tag{2}$$

where

$$\begin{aligned} X_{\mathbf{i}} &= \sum_{\mathbf{q}} \sqrt{\left(\frac{\hbar}{2NM\omega_{\mathbf{q}}} \right)} (a_{\mathbf{q}} + a^+_{-\mathbf{q}}) e^{i\mathbf{q}\cdot\mathbf{R_i}} \\ P_{\mathbf{i}} &= i \sum_{\mathbf{q}} \sqrt{\left(\frac{\hbar M\omega_{\mathbf{q}}}{2N} \right)} (a^+_{\mathbf{q}} - a_{-\mathbf{q}}) e^{-i\mathbf{q}\cdot\mathbf{R_i}} \end{aligned} \tag{3}$$

denote the operators describing electron-phonon coupling induced local lattice deformations and shifts in the electron momenta respectively.

Quite generally, in polaronic systems two parameters are controlling their physics: (i) the strength of electron lattice coupling $\alpha = \varepsilon_P/\hbar\bar{\omega}$ ($\bar{\omega}$ denoting some averaged phonon frequency and ε_P the polaron energy level shift) and the adiabaticity ratio $t/\bar{\omega}$ (t denoting the bare electron hopping integral defining the electron dispersion $\varepsilon_{\mathbf{k}} = \frac{t}{z} \sum_{\delta} e^{i\mathbf{k}\cdot\delta}$, z being the coordination number and δ the lattice vectors linking nearest neighbor sites. Let us now consider two limiting cases of such unitary transformations in terms of these parameters.

A. Weak coupling adiabatic limit

In this case we can restrict ourselves to states consisting of electrons accompanied by not more than a single phonon at any given time and thus can limit ourselves to terms in the tranformed Hamiltonian being of quadratic order in $V_{\mathbf{q}}$. This imposes the condition $[H_{\rm el}, S]_- + H_{\rm ph} = 0$ which determines the parameters π and χ

$$\begin{aligned} \pi_{(j-i,\, l-i)} &= [\pi^+_{(j-i,\, l-i)} - \pi^-_{(j-i,\, l-i)}],\ \chi_{(j-i,\, l-i)} = [\chi^+_{(j-i,\, l-i)} + \chi^-_{(j-i,\, l-i)}] \\ \chi^{\pm}_{(j-i,\, l-i)} &= \frac{1}{2N} \sum_{\mathbf{k}\,\mathbf{q}} \frac{V_{\mathbf{q}}}{\varepsilon_{\mathbf{k}} - \varepsilon_{\mathbf{k-q}} \mp \hbar\omega_{\mathbf{q}}} \sqrt{\left(\frac{2M\omega_{\mathbf{q}}}{\hbar} \right)} e^{i\mathbf{k}\cdot(\mathbf{R}_j - \mathbf{R}_i)} e^{i\mathbf{q}\cdot(\mathbf{R}_i - \mathbf{R}_l)} \\ \pi^{\pm}_{(j-i,l-i)} &= \frac{1}{2iN} \sum_{\mathbf{k}\,\mathbf{q}} \frac{V_{\mathbf{q}}}{\varepsilon_{\mathbf{k}} - \varepsilon_{\mathbf{k-q}} \mp \hbar\omega_{\mathbf{q}}} \sqrt{\left(\frac{2}{M\hbar\omega_{\mathbf{q}}} \right)} e^{i\mathbf{k}\cdot(\mathbf{R}_j - \mathbf{R}_i)} e^{i\mathbf{q}\cdot(\mathbf{R}_i - \mathbf{R}_l)}. \end{aligned} \tag{4}$$

The resulting effective Hamiltonian is

$$\tilde{H}_{\rm BCS} = \sum_{\mathbf{k}\sigma}(\varepsilon_{\mathbf{k}} - \mu)c^{+}_{\mathbf{k}\sigma}c_{\mathbf{k}\sigma}$$
$$+ \sum_{\mathbf{k}\mathbf{k}'\mathbf{q}} |V_{\mathbf{q}}|^2 c^{+}_{\mathbf{k}+\mathbf{q}\uparrow}c^{+}_{\mathbf{k}'-\mathbf{q}\downarrow}c_{\mathbf{k}'\downarrow}c_{\mathbf{k}\uparrow}\frac{\hbar\omega_{\mathbf{q}}}{(\varepsilon_{\mathbf{k}} - \varepsilon_{\mathbf{k}-\mathbf{q}})^2 - (\hbar\omega_{\mathbf{q}})^2} \tag{5}$$

which is nothing but the BCS Hamiltonian. The phyiscs which is behind this transformation can be seen by looking at the transformed electron operators in real space, i.e.,

$$\tilde{c}^{+}_{\mathbf{m}\sigma} = c^{+}_{\mathbf{m}\sigma} + \sum_{\mathbf{i}\,\mathbf{l}} c^{+}_{\mathbf{i}\sigma}[\pi_{(m-i,\, l-i)}P_{\mathbf{l}} + \chi_{(m-i,\, l-i)}X_{\mathbf{l}}]. \tag{6}$$

$\pi_{(m-i,\, l-i)}$ and $\chi_{(m-i,\, l-i)}$ are slowly varying functions of $\mathbf{R}_m - \mathbf{R}_i$ which extend over large distances of the order of $1/\delta k \simeq (2a/\pi)(v_F/s)$, given the fact that $\mathbf{k}$ in the expressions for π and χ are restricted to a thin region around $\mathbf{k_F}$ controlled by an average phonon energy $s\pi/a$ (a denoting the lattice constant and v_F the Fermi velocity). $\pi_{(m-i,\, l-i)}$ and $\chi_{(m-i,\, l-i)}$ on the contrary are relatively strongly peaked functions around $\mathbf{R_l} - \mathbf{R_i} = 0$ since the phonon wave vectors $\mathbf{q}$ in the expressions for π and χ connect any two points on the Fermi surface and thus cover a wide interval, $[0, 2k_F]$.

This leads to (see fig. 1):
(i) dynamical deformations of the lattice around the sites $\mathbf{l}$ (controlled by $\pi_{(m-i,\, l-i)}$), caused by the presence of the electron between sites $\mathbf{m}$ and $\mathbf{i}$ some distance away from site $\mathbf{l}$
(ii) induce a propagating motion of the ionic deformations at sites $\mathbf{l}$ (controlled by $\chi_{(m-i,\, l-i)}$) through the crystal by transferring part of the momentum of the electron to the lattice.

Given the fact that $v_F \gg s$, the dynamical lattice derformation surrounding the itinerant electrons can be considered as static. An electron moving in the lattice trails with it a lattice deformation in a kind of tube[11] without radiating off this deformation into the crystal as a whole. A second electron, coming from the opposite direction, can absorb such a primary lattice deformation and it is this which leads to the effective electron-electron attraction which is at the heart of the BCS mechanism for Cooper-pair formation.

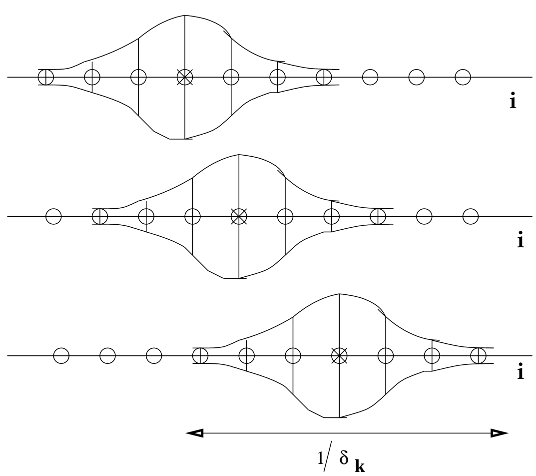

FIG. 1: Schematic representation of the transformed electron charge and lattice displacements for three successive time steps of the electron moving from site to site and characterized by (i) a delocalization of the electron over a distance $1/\delta_{\mathbf{k}}$ controlled by the range of the induced deformation centered at a site $\mathbf{m}$ and indicated by the filled circle, (ii) an amplitude modulated dynamical lattice deformation.

B. Strong coupling anti-adiabatic limit

In that case the electron energies $\varepsilon_{\mathbf{k}}$ in the denominator of the expressions for π and χ can be treated in a perturbative way. We can furthermore assume the phonons as being given by dispersion-less Einstein modes with frequency ω_0 and a corresponding electron-phonon coupling $V_{\mathbf{q}} = \lambda\sqrt{\hbar/2M\omega_0}$. To lowest order in $\varepsilon_k/\hbar\omega_0$ this yields:

$$\chi_{(m-i,\, l-i)} = 0 \quad \text{and} \quad \pi_{(m-i,\, l-i)} = (i\lambda/\hbar M\omega_0^2)\delta_{im}\delta_{il}.$$

Treating $\varepsilon_k/\hbar\omega_0$ in a perturbative way reproduces the results amounting to the Lang Firsov transformation[12] for small polarons, with the operator S reducing to

$$S_{\rm LF} = \sum_{\mathbf{i}\,\sigma} c^{+}_{\mathbf{i}\sigma}c_{\mathbf{i}\sigma}\pi_{(0,0)}P_{\mathbf{i}} = -\alpha\sum_{\mathbf{i}\,\sigma} c^{+}_{\mathbf{i}\sigma}c_{\mathbf{i}\sigma}(a_{\mathbf{i}} - a^{+}_{\mathbf{i}}) \tag{7}$$

and with $\alpha = \frac{\lambda}{\sqrt{2\hbar M\omega_0^3}}$. The operator $S_{\rm LF}$ transforms the initial electron on site $\mathbf{i}$ into an electron surrounded by a local lattice deformation

$$\tilde{c}^+_{\mathbf{i}\sigma} = c^+_{\mathbf{i}\sigma} X^+_{\mathbf{i}},\ X^+_{\mathbf{i}}|0) = e^{-\alpha(a_{\mathbf{i}} - a^+_{\mathbf{i}})}|0) = \sum_n e^{-\frac{1}{2}\alpha^2} \frac{(\alpha)^n}{\sqrt{n!}}|n)_{\mathbf{i}}. \tag{8}$$

H transforms correspondingly into an effective polaron Hamiltonian

$$\begin{aligned}\tilde{H} &= \sum_{\mathbf{i}\,\sigma}(D-\varepsilon_P)c^+_{\mathbf{i}\sigma}c_{\mathbf{i}\sigma} - t\sum_{\mathbf{i}\neq\mathbf{j},\sigma}(c^+_{\mathbf{i}\sigma}c_{\mathbf{j}\sigma}X^+_{\mathbf{i}}X^-_{\mathbf{j}} + H.c.)\\ &- \ 2\varepsilon_P\sum_{\mathbf{i}}c^+_{\mathbf{i}\uparrow}c^+_{\mathbf{i}\downarrow}c_{\mathbf{i}\downarrow}c_{\mathbf{i}\uparrow} + \hbar\omega_0\sum_{\mathbf{i}}(a^+_{\mathbf{i}}a_{\mathbf{i}} \ + \frac{1}{2}),\end{aligned} \tag{9}$$

whose main physical features have been discussed in my Introductory lecture "Introduction to polaron physics: Basic Concepts and models" in this volume and where ε_P denotes the polaron ionization energy.

In the limit $2\varepsilon_P > D$ (D denoting the band half-width), bipolaronic states are stable, i.e., the ionization energy of two polarons on different sites ($2\varepsilon_P$) is smaller than of two electrons on a single site ($4\varepsilon_P$). Approximating the effective electron hopping term by

$$tc^+_{\mathbf{i}\sigma}c_{\mathbf{j}\sigma}X^+_{\mathbf{i}}X^-_{\mathbf{j}} \to t^* c^+_{\mathbf{i}\sigma}c_{\mathbf{j}\sigma}, \tag{10}$$

with $t^* = te^{-\alpha^2}$ (the Lang-Firsov approximation[12], appropriate for that anti-adiabatic strong coupling case) we subsequently eliminate all singly occupied sites via a unitary transformation given by

$$(S_{\rm BP})_{\alpha\beta} = \sum_{\mathbf{i}\neq\mathbf{j}} \frac{(t^*)^2(c^+_{\mathbf{i}\sigma}c_{\mathbf{j}\sigma})_{\alpha\beta}}{E_\alpha - E_\beta}. \tag{11}$$

The relevant matrix elements link empty and doubly occupied sites on nearest neighbors with singly occupied ones and E_α, E_β denote the energies of single site states of $\tilde{H}$ in the limit $t = 0$. The resulting transformed Hamiltonian describes a system of itinerant Bipolarons on a lattice[10] and is given by

$$H_{\rm BP} = e^{-S_{\rm BP}}\tilde{H}e^{S_{\rm BP}} = -\sum_{\mathbf{i}} 2(\varepsilon_P - \mu)(\rho^z - \frac{1}{2}) - \frac{(t^*)^2}{2\varepsilon_P}\sum_{<\mathbf{i}\neq\mathbf{j}>}(\rho^+_{\mathbf{i}}\rho^-_{\mathbf{j}} + H.c.). \tag{12}$$

This corresponds to an effective pseudo-spin-$\frac{1}{2}$ X-Y model in an external field, given the fact that Bipolarons are hard core bosons having spin-$\frac{1}{2}$ statistics with

$$\rho^+_{\mathbf{i}} = c^+_{\mathbf{i}\uparrow}c^+_{\mathbf{i}\downarrow}, \quad \rho^-_{\mathbf{i}} = c_{\mathbf{i}\downarrow}c_{\mathbf{i}\uparrow},\ \rho^z_{\mathbf{i}} = \frac{1}{2} - \rho^+_{\mathbf{i}}\rho^-_{\mathbf{i}} \tag{13}$$

$$[\rho^-_{\mathbf{i}}, \rho^+_{\mathbf{i}}]_+ = 1,\ [\rho^-_{\mathbf{i}}, \rho^+_{\mathbf{i}}]_- = \frac{1}{2} - \rho^+_{\mathbf{i}}\rho^-_{\mathbf{i}},\ [\rho^-_{\mathbf{i}}, \rho^+_{\mathbf{j}}]_- = 0\ (\mathbf{i}\neq\mathbf{j}) \tag{14}$$

This is a description analogous to that introduced by Anderson's pseudospin representation[8] of the effective BCS Hamiltonian, eq. (5), when restricting Cooper pairing to zero momentum pairs, resulting in:

$$H_{\rm BCS} = -\sum_{\mathbf{k}}(\varepsilon_{\mathbf{k}} - \mu)(\tau^z_{\mathbf{k}} - \frac{1}{2}) - \sum_{\mathbf{k}\mathbf{k}'} v(\mathbf{k}, \mathbf{k}')(\tau^+_{\mathbf{k}}\tau^-_{\mathbf{k}'} + H.c.). \tag{15}$$

$H_{\rm BCS}$ has a structure which is formally similar to that of the Hamiltonian for Bipolarons $H_{\rm BP}$, except that here it is in $\mathbf{k}$-space rather than in real space and with corresponding pseudospin-$\frac{1}{2}$ operators

$$\tau^+_{\mathbf{k}} = c^+_{\mathbf{k}\uparrow}c^+_{-\mathbf{k}\downarrow}, \quad \tau^-_{\mathbf{k}} = c_{-\mathbf{k}\downarrow}c_{\mathbf{k}\uparrow},\ \tau^z_{\mathbf{k}} = \frac{1}{2} - \tau^+_{\mathbf{k}}\tau^-_{\mathbf{k}} \tag{16}$$

$$[\tau^-_{\mathbf{k}}, \tau^+_{\mathbf{k}}]_+ = 1,\ [\tau^-_{\mathbf{k}}, \tau^+_{\mathbf{k}}]_- = \tau^z_{\mathbf{k}},\ \ [\tau^-_{\mathbf{k}}, \tau^-_{\mathbf{k}'}]_- = 0\ (\mathbf{k}\neq\mathbf{k}'). \tag{17}$$

C. Macroscopic phase-locking in superconductivity

The ground states of those two limiting cases of the electron-lattice interaction considered above are phase correlated states of the form

$$\Psi^0_{BP} = \prod_{\mathbf{i}} (u_{\mathbf{i}} e^{(\frac{i\phi_{\mathbf{i}}}{2})} + v_{\mathbf{i}} e^{(-\frac{i\phi_{\mathbf{i}}}{2})} \rho^+_{\mathbf{i}})|0\rangle \tag{18}$$

$$\Psi^0_{BCS} = \prod_{\mathbf{k}} (u_{\mathbf{k}} e^{(\frac{i\phi_{\mathbf{k}}}{2})} + v_{\mathbf{k}} e^{(-\frac{i\phi_{\mathbf{k}}}{2})}) \tau^+_{\mathbf{k}}|0\rangle \tag{19}$$

where $u_{\mathbf{i}}, v_{\mathbf{i}}, \phi_{\mathbf{i}}$ and $u_{\mathbf{k}}, v_{\mathbf{k}}, \phi_{\mathbf{k}}$ denote the local amplitudes and phases of the Bipolarons and Cooperons respectively and which, in a macroscopic coherent quantum state describing a homogeneous superconducting ground state, have to be independent on the sites $\mathbf{i}$ and respectively the wave vectors $\mathbf{k}$. Superconductivity corresponds to an off-diagonal long range order with components of the pseudo-spins which are aligned ferro-magnetically in the $x - y$ plane. The modulus of these $x - y$ components determine the amplitude of the order parameter. The z-component of the pseudo-spins determine the density of Bipolarons, respectively of Cooperons. The quantification axes of those pseudo-spins being arbitrary but fixed, is chosen here according to the presentation in fig. 2. These variational mean field

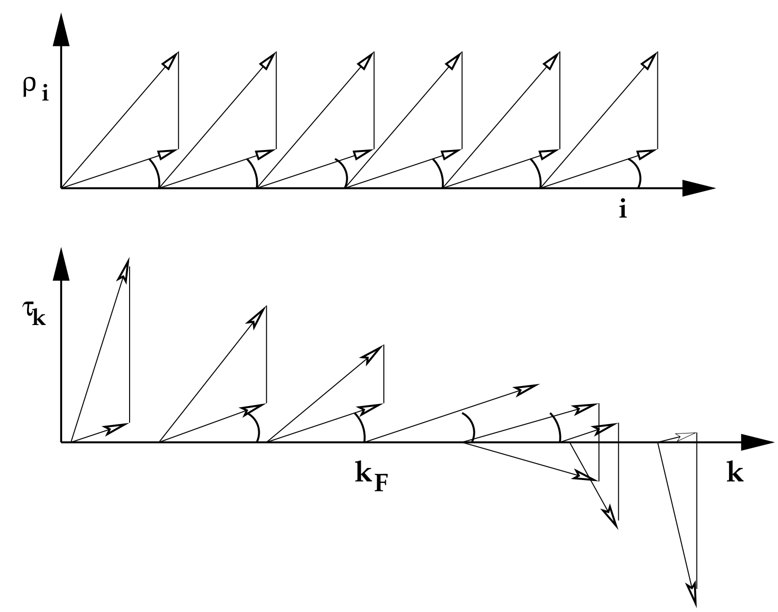

FIG. 2: The pseudospin representation of the superconducting ground state, manifest in the alignement of the basal plane components of the pseudospin vectors indicative of long range phase coherence in the strong coupling Bipolaronic (top figure) and the weak coupling BCS (bottom figure) limit.

solutions for the superconducting ground states for those two extreme limiting cases, eqs. (18,19) have distinctively and qualitatively different excitation spectra which can be easily visualized by inspection of fig. 2. For the case of Bipolarons, the dominant excitations are collective modes which correspond to pseudo-magnons and where, to lowest order, amplitude fluctuations play no role. This indicates a temperature driven transition from the superconducting into a normal state where Bipolarons continue to exist above the superconducting critical temperature T_c up to around a certain temperature T^*. Above T^* they very rapidly break up into individual electrons and the amplitude of the order parameter, even on a short time scale, disappeares. For the case of Cooper pairs, the dominant excitations which control the breakdown of superconductivity are amplitude fluctuations near the Fermi surface which break down the k-space pairing and hence cause the vanishing of the amplitude of the order parameter. The breakdown of any long range phase correlations is here just a natural consequence of the vanishing of the amplitude of the order parameter.

The temperature which controls the break-down of these two superconducting phases are given respectively by the binding energy of Cooper-pairs (determined by the zero temperature energy gap Δ_0) and the phase stiffness of the

condensate of the Bipolarons D_ϕ multiplied by their correlation length ξ:

$$\Delta_0 \simeq 2\hbar < \omega_{\mathbf{q}} > e^{-\frac{1+\Lambda}{\Lambda}},\ \Lambda = N(0)\frac{< v^2(\mathbf{k},\mathbf{k}') >}{< \omega_{\mathbf{q}}^2 >}, \tag{20}$$

$$D_\phi = \hbar^2(n_{\rm BP}/m_{\rm BP}). \tag{21}$$

$< ... >$ denote appropriately chosen averages over the Fermi surface of the phonon frequencies and the electron-lattice couplings. $n_{\rm BP}$ denotes the density of the Bipolarons and $m_{\rm BP} \simeq (e^{2\alpha^2}/2\alpha^2\hbar\omega_0)m_{\rm el}$ ($m_{\rm el}$ denoting the bare electron band mass) their exceedingly heavy mass[10], which makes the chances of ever finding such a superconducting state extremely slim. Bipolaronic superconductivity definitely is not an explanation for the recently discovered high T_c cuprate superconductors[13] which fall in the cross-over regime between BCS and Bipolaronic superconducivity and are characterized by Fermionic rather than Bosonic quasi-particles in the normal state.

III. RESONATING BIPOLARONS

As we have seen above, as a function of strength of the electron-phonon coupling and the adiabaticity ratio, we can obtain two qualitatively distinct superconducting phases:
(i) a BCS like phase controlled by amplitude fluctuations in the weak coupling adiabatic limit,
(ii) a Bipolaronic Superconductor phase, controlled by phase fluctuations of tightly bound electron pairs in the strong coupling anti-adiabatic limit when the attractive interaction between two electrons is big enough such as to form true bound states (with a binding energy $\varepsilon_{BP} = 4\alpha^2\hbar\omega_0 > 2D$) below the continuum of the itinerant electronic states (see fig. 3a).

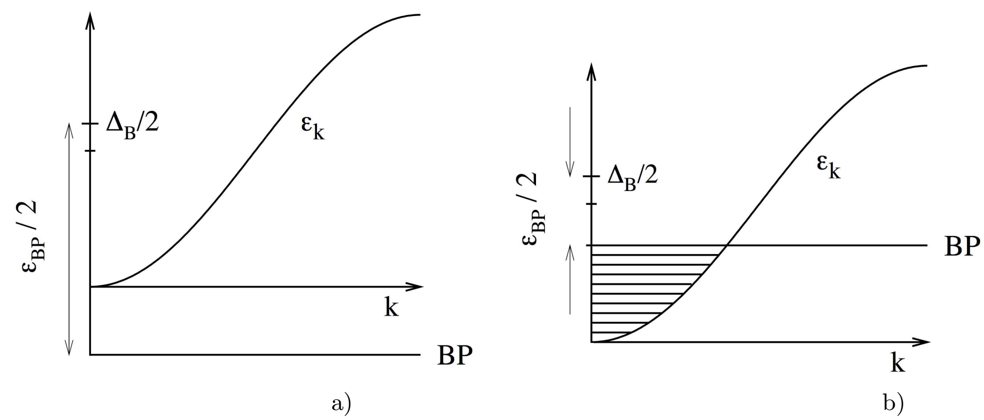

FIG. 3: Schematic plot of the bipolaron level (BP) falling below the band of itinerant electrons (a) and inside this band (b).

Let us now consider the situation when the binding energy $\varepsilon_{\rm BP}$ of two electrons, dynamically decoupled from the rest of the remaining charge carriers in the system, is less than the band width $2D$. In that case we have an overlapp in energy of such localized locally bound pairs and the non-interacting itinerant electrons (see fig. 4), which will give rise to resonant scattering between the two species. On the basis of such a simple intuitive picture and as a follow-up of the Bipolaronic Superconductor scenario[10], a phenomenological model was proposed in the early eighties—the Boson-Fermion model—devised to capture the main features of electron-lattice coupled systems in the cross-over regime between weak and strong coupling. The corresponding Hamiltonian for that is given by[14,15]:

$$\begin{aligned} H_{\rm BFM} &= (D-\mu)\sum_{\mathbf{i},\sigma} n_{\mathbf{i}\sigma} - t\sum_{\langle \mathbf{i}\neq\mathbf{j}\rangle\sigma} c^+_{\mathbf{i}\sigma}c_{\mathbf{j}\sigma} \\ &\quad -(\Delta_B - 2\mu)\sum_{\mathbf{i}}\left(\rho^z_{\mathbf{i}} - \frac{1}{2}\right) + v\sum_{\mathbf{i}}[\rho^+_{\mathbf{i}}c_{\mathbf{i}\downarrow}c_{\mathbf{i}\uparrow} + \rho^-_{\mathbf{i}}c^+_{\mathbf{i}\uparrow}c^+_{\mathbf{i}\downarrow}] \\ &\quad -\hbar\omega_0\alpha\sum_{\mathbf{i}}\left(\rho^z_{\mathbf{i}} - \frac{1}{2}\right)(a_{\mathbf{i}} + a^+_{\mathbf{i}}) + \hbar\omega_0\sum_{\mathbf{i}}\left(a^+_{\mathbf{i}}a_{\mathbf{i}} + \frac{1}{2}\right). \end{aligned} \tag{22}$$

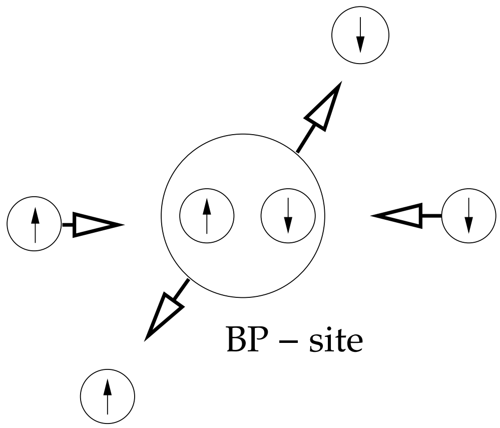

FIG. 4: Schematic plot of a resonant process of localized Bipolarons and pairs of itinerant electrons.

$\rho^+_{\mathbf{i}}, \rho^-_{\mathbf{i}}, \rho^z_{\mathbf{i}}$ denote creation, annihilation, and density operators for localized electron pairs coupled to local lattice deformations and which, as a result of that coupling, end up as localized Bipolarons described by $\rho^+_{\mathbf{i}}\, X^+_{\mathbf{i}} \equiv c^+_{\mathbf{i}\uparrow}\, c^+_{\mathbf{i}\downarrow}\, e^{-2\alpha(a_{\mathbf{i}}\; - a^+_{\mathbf{i}})}$. We subsequently treat such localized Bipolarons as commuting with the itinerant electrons but compensate that transgression by introducing phenomenologically a charge exchange term of strength v between the two species. Experimental tests which go along with such a scenario are based on measurements of local structural dynamical instabilities which show up in pair distribution functions consisting of a double peak structure which strongly depends on the time scale of the experiments (see the articles by T. Egami and N. Saini, this volume). The manifestation of a double peak structure of the local lattice environment is a consequence of local lattice deformation fluctuation induced by the resonant pairing of the itinerant electrons on polaronic sites[14]. This goes hand in hand with the evoltion of spectral features in the two-particle properties which go from well defined itinerant behavior (characterized by a sharp peak at a given frequency for a specific $\mathbf{k}$ vector) to that of localized features (characterized by a broad incoherent background). The resonant behavior which lies between these two limiting cases is characterized by a spectral function where those two features overlap in frequency.

Treating the cross-over regime of the electron-lattice coupled systems on the basis of this Boson-Fermion model introduces a separation of energy scales according to which electron-pair correlations start to build up independently of any superconducting long range order. But unlike the strong coupling limit, where the state above the superconducting state is one of itinerant Bipolarons, here, the normal state is a system of electrons which due to their strong lattice induced attractive interaction show a well pronounced pseudogap. This pseudogap only disappears at much higher temperature, when finally these local electron-pair correlations disappear. The lattice induced origin for pairing giving rise to superconductivity in such a scenario can be examined via the isotope effect, not of the onset temperature of superconductivity but rather of the onset temperature of electron-pair correlations. Although these correlations are dynamical in origin and do not show up as a phase transition at a given temperature, their onset is very abrupt around a certain temperature T^*. One thus can get a reasonably good indication for the isotope effect of electron pairing around T^* by studying this model within a mean field analysis[16] which determines T^* as being exclusively due to amplitude fluctuations of the electron-pairs. Given this situation we can formulate a variational state as the direct product of the two components involving localized Bipolarons and pairs of itinerant electrons: $|\Psi^{\rm F}\rangle \otimes \prod_{\mathbf{i}} |\; l\; \}^B_{\mathbf{i}}$ with

$$|\Psi^{\rm F}\rangle = \prod_{\mathbf{k}} \Big[u_{\mathbf{k}} + v_{\mathbf{k}} c^+_{\mathbf{k}\uparrow} c^+_{-\mathbf{k}\downarrow} \Big] |0\rangle, \quad |\; l\; \}^B_{\mathbf{i}} = \sum_n \big[u_{ln}(i) + v_{ln}(i)\, \rho^+_{\mathbf{i}} \big] |0)_{\mathbf{i}} |n >_{\mathbf{i}} \;\; . \tag{23}$$

$|n >_{\mathbf{i}}$ denotes the set of oscillator states on sites $\mathbf{i}$ composed of n phonons. The exchange coupling term in $H_{\rm BFM}$, eq. (22) then becomes

$$v\rho x + vx \sum_{\mathbf{i}} [\rho^+_{\mathbf{i}} + \rho^-_{\mathbf{i}}] + \frac{v\rho}{2} \sum_{\mathbf{k}} [c_{-\mathbf{k}\downarrow} c_{\mathbf{k}\uparrow} + c^+_{\mathbf{k}\uparrow} c^+_{-\mathbf{k}\downarrow}] \tag{24}$$

with

$$x \;=\; \frac{1}{N} \sum_{\mathbf{i}} \langle c^+_{\mathbf{i}\uparrow} c^+_{\mathbf{i}\downarrow} \rangle\,, \quad \rho \;=\; \frac{1}{N} \sum_{\mathbf{i}} \langle \rho^+_{\mathbf{i}} + \rho^-_{\mathbf{i}} \rangle \tag{25}$$

denoting the amplitudes of the order parameters of the electron and Bipolaron subsystems. The corresponding mean

field Hamiltonian thus reduces to

$$
\begin{aligned}
H_{\mathrm{MFA}} &= H_F + H_B - v\rho x + \frac{\hbar\omega_0}{2} \\
H_F &= (D-\mu)\sum_{\mathbf{i},\sigma} c^+_{\mathbf{i}\sigma} c_{\mathbf{i}\sigma} - t \sum_{\langle \mathbf{i}\neq\mathbf{j}\rangle,\sigma} c^+_{\mathbf{i}\sigma} c_{\mathbf{j}\sigma} \\
&\quad + \frac{v\rho}{2}\sum_{\mathbf{i}}[c_{\mathbf{i}\downarrow}c_{\mathbf{i}\uparrow} + c^+_{\mathbf{i}\uparrow}c^+_{\mathbf{i}\downarrow}] \\
H_B &= -(\Delta_B - 2\mu)\sum_{\mathbf{i}}\left(\rho^z_{\mathbf{i}} - \frac{1}{2}\right) + vx\sum_{\mathbf{i}}[\rho^+_{\mathbf{i}} + \rho^-_{\mathbf{i}}] \\
&\quad - \hbar\omega_0\alpha\sum_{\mathbf{i}}\left(\rho^z_{\mathbf{i}} - \frac{1}{2}\right)(a_{\mathbf{i}} + a^+_{\mathbf{i}}) + \hbar\omega_0\sum_{\mathbf{i}}(a^+_{\mathbf{i}}a_{\mathbf{i}} + \frac{1}{2})\,. \qquad (26)
\end{aligned}
$$

with mean field equations for the order parameters given by

$$
\begin{aligned}
x &= -\frac{v\rho}{4N}\sum_{\mathbf{k}} \frac{1}{\tilde{\epsilon}_{\mathbf{k}}(\rho)} \tanh\frac{\beta\tilde{\epsilon}_{\mathbf{k}}(\rho)}{2}\,, \\
\rho &= \frac{1}{Z}\sum_{ln} u_{ln}\, v_{ln}\, \exp\left[-\beta E_l(x)\right]\,, \\
n_{tot} &= \frac{1}{4}\rho^2 + 2 - \frac{1}{N}\sum_{\mathbf{k}}\left(\frac{\varepsilon_{\mathbf{k}}}{\tilde{\varepsilon}_{\mathbf{k}}(\rho)} \tanh\frac{\beta\tilde{\varepsilon}_{\mathbf{k}}(\rho)}{2}\right) \\
&\quad + \frac{1}{Z}\sum_{ln}\left[(u_{ln})^2 - (v_{ln})^2\right]\exp\left[-\beta E_l(x)\right]. \qquad (27)
\end{aligned}
$$

$Z = \sum_l e^{-\beta E_l(x)}$ denotes the partition function corresponding to the bosonic part of the mean-field Hamiltonian. Such a procedure describes the opening of a true gap of size $v\rho$ in the single-particle electron spectrum $\tilde{\varepsilon}_{\mathbf{k}}(\rho) = \pm\sqrt{(\varepsilon_{\mathbf{k}} - \mu)^2 + (v\rho)^2/4}$, but under the present physical circumstances should be taken as a qualitative description for the real situation where it is a pseudogap rather than a true gap which opens up at T^*[17]. This pseudogap plays the role of a precursor to a true superconducting state at some lower temperature which is controlled by phase fluctuations[18]. Such a scenario was indeed experimentally veryfied in the high T_c cuprate superconductors[19] shortly after this theoretical prediction.

Solving the selfconsistent set of eqs. (27) for T^* (alias the mean field critical temperature) for different values of phonon frequencies ω_0 and for a set of concentrations of electrons and localized Bipolarons, we illustrate in fig. 5 its dependence on ω_0. The isotope effect in classical weak coupling BCS superconductors is defined by an exponent α which relates the critical temperature for superconductivity to the mass of the ions (alternatively to the phonon frequency) via $T_c \propto \omega_0^\alpha$ and with a value for α generally around 0.5. In the present scenario, in contrast, the isotope coefficent for T^* itself varies as a function of ω_0. The corresponding isotope exponent then has to be defined by the relation

$$
\alpha^* = 0.5\ \ln\left(\frac{T^*(i)}{T^*(i+1)} / \frac{\omega_0(i)}{\omega_0(i+1)}\right). \qquad (28)
$$

where $\omega_0(i), T^*(i)$ denote a set of different, closely lying together, values of phonon frequencies and hence correponding temperatures for the onset of pair-corellations. α^* approaches constant positive values in the BCS-like limit where Bipolarons are only virtually excited but its value still depends sensitively on ω_0. In the case where we have a mixture of itinerant electrons and localized Bipolarons (the case for which this model has been designed) the isotope exponent deviates significantly from any BCS like behavior. It shows negative and large values which, for the set of parameters chosen in fig. 5, fall typically between -0.5 and -1. There are strong experimental indications for such large negative values of α^* in a number of high T_c cuprates. Experiments measuring T^* must be fast enough to capture two electrons remaining correlated over a finite time, which is typically of the order of the vibrational frequency of local modes ($\simeq 10^{-13} - 10^{-15}$ sec), such as to give rise to Bipolaron formation. Neutron spectroscopy, studying the relaxation rate of crystal field excitations and XANES (X-ray absorption near edge spectroscopy) as well as EXAFS are in the right range of time scale and have given results in a number of high T_c cuprates[20] such as $La_{2-x}Sr_xCuO_4$, Ho Ba_2Cu_4 O_8 and $La_{1.81}Ho_{0.04}Sr_{0.15}CuO_4$.

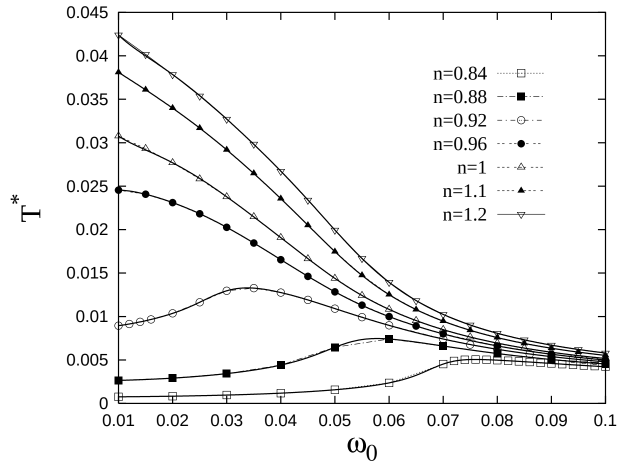

FIG. 5: T^* as a function of ω_0 for $\alpha = 2$ and $v = 0.25$ (after ref. [16]).

IV. LOCAL VERSUS NON LOCAL PHASE COHERENCE IN THE BOSON-FERMION MODEL

In sections II and III above we have shown that the amplitude of the order parameter controls in quite analogous fashions, (i) the onset of superconductivity in BCS-like systems and (ii) the onset of electron pairing, but without any superconductivity, in systems which are in the cross-over regime between a BCS superconductor and a superfluid state of tightly bound electron-pairs. The physics leading to the onset of superconductivity in such a cross-over regime is a subject which presently is far from being completely understood. What does emerge however from preliminary studies is that the onset of a condensed superfluid state of Bipolaronic bosons has a strong effect on the lattice and generally leads to its stiffening, as several examples show: (i) non-interacting itinerant charged bosons coupled to acoustic longitudinal phonons manifest an abrupt change in the increase of sound velocity as the temperature is reduced to below the condensation temperature of the bosons[21], (ii) the coupling of weakly interacting itinerant bosons to local Einstein modes on a deformable lattice results in correlated condensates involving both, the bosons as well as the phonons[24], (iii) localized Bipolarons coupled to a system of itinerant electrons, such as described by the Boson Fermion model scenario, leads to an abrupt change in the decrease of the Debye Waller factor as the temperature decreases through T^*[15,25]. All these preliminary indications for strong electron-phonon coupling induced macroscopic lattice effects (particularly well documented in the study of the high T_c cuprate superconductors) can possibly be the reason for: (i) the onset of dynamically ordered vibrations of atoms upon entering the superfluid phase, such as seen in Rutherford back scattering experiments[26], (ii) the abrupt changes in the decrease of the kinetic energies of the atomic vibrations[27], (iii) changes in the near IR excited Raman scattering structure showing an abrupt increase in the low energy electronic background[28], (iv) a sharp increase in the intensity of certain Raman active phonon modes suggesting a modification of the scattering mechanism[29] as well as (v) similar abrupt changes in the sound velocity of certain modes and the Debye Waller factors (we refer the reader to the articles by Egami and Saini in this volume).

Let us conclude this overview of resonating Biplolarons by a discussion of their superfluid properties and the possibility of a Superconductor - Bipolaron Insulator quantum phase transition. Such physics goes beyond the so-called BCS to local pair superconductor cross-over which has been widely studied in the past[30,31,32] on the basis of models with an effective attractive interaction between the electrons. These studies invariably show a continuous evolution of a superfluid ground state as the strength of this interaction is varied. What is new in the present scenario is that the locally fluctuating lattice deformations—which we believe to be the main new feature in this cross-over regime of electron-lattice coupled systems—lead to strong local correlations between two types of charge carriers: itinerant electrons and localized bound electron-pairs which resonate on a given polaronic site. It is this mechanism which not only incites pairing of the itinerant electrons and their ultimate superfluid features but also limits their long range superfluid phase correlations when this exchange coupling goes beyond a certain critical value. In order to reduce the complexity of this problem let us now assume the phonons in the clouds surrounding the locally bound pairs to be frozen out. This amounts to consider the case of a mixture of tightly bound localized electron-pairs (localized Bipolarons where the lattice deformations surrounding those charge carriers are static) which are exchange-coupled

to pairs of itinerant electrons. The corresponding reduced Boson-Fermion model is then given by

$$\begin{aligned} H_{\rm BFM} &= (D-\mu)\sum_{\mathbf{i}\sigma} c^+_{\mathbf{i}\sigma}c_{\mathbf{i}\sigma} - t\sum_{<\mathbf{i},\mathbf{j}>\sigma} c^+_{\mathbf{i}\sigma}c_{\mathbf{j}\sigma} - (\Delta_B - 2\mu)\sum_{\mathbf{i}}(\rho^z_{\mathbf{i}} - \frac{1}{2}) \\ &+ \; g\sum_{\mathbf{i}}(\rho^+_{\mathbf{i}}\tau^-_{\mathbf{i}} + (\rho^-_{\mathbf{i}}\tau^+_{\mathbf{i}}) \end{aligned} \tag{29}$$

where g denotes some effective exchange coupling constant. $\{\rho^+_{\mathbf{i}}, \rho^-_{\mathbf{i}}, \rho^z_{\mathbf{i}}\}$ denote, as before, localized tightly bound electron-pairs and

$$\tau^+_{\mathbf{i}} = c^+_{\mathbf{i}\uparrow}c^+_{\mathbf{i}\downarrow}, \quad \tau^-_{\mathbf{i}} = c_{\mathbf{i}\downarrow}c_{\mathbf{i}\uparrow}, \quad \tau^z_{\mathbf{i}} = \frac{1}{2} - \tau^+_{\mathbf{i}}\tau^-_{\mathbf{i}} \tag{30}$$

$$[\tau^-_{\mathbf{i}}, \tau^+_{\mathbf{i}}]_+ = 1, \; [\tau^-_{\mathbf{i}}, \tau^+_{\mathbf{i}}]_- = \tau^z_{\mathbf{i}}, \; [\tau^-_{\mathbf{i}}, \tau^-_{\mathbf{j}}]_- = 0 \; (\mathbf{i} \neq \mathbf{j}) \tag{31}$$

pairs of itinerant electrons in real space which are the equivalents of the Cooper-pairs $\{\tau^+_{\mathbf{k}}, \tau^-_{\mathbf{k}}, \tau^z_{\mathbf{k}}\}$ in the standard BCS scenario discussed in section II B. In order to illustrate the competition between local and global phase coherence let us consider for simplicity's sake and without any loss of generality the case $\Delta_B = 0, \mu = 0, n_F = n_B = 1$. In the limit where the itinerancy of the electrons can be neglected against the pair-exchange coupling, $t << g$, the ground state is given by

$$\prod_{\mathbf{i}} \frac{1}{\sqrt{2}} e^{i\phi_{\mathbf{i}}}[\rho^+_{\mathbf{i}} + \tau^+_{\mathbf{i}}]|0> . \tag{32}$$

It presents an insulating system of locally strongly correlated pairs involving the two species of charge carriers, with full phase locking between them but arbitrary and thus uncorrelated local phases $\phi_{\mathbf{i}}$ on different sites. With decreasing g/t one should expect that the above state goes over into a superfluid phase locked state with $\phi_{\mathbf{i}} \equiv \phi$ which, to within the simplest approximation, could be assumed by the form

$$\prod_{\mathbf{i}} (u + v\rho^+_{\mathbf{i}}|0> \otimes (u' + v'\tau^+_{\mathbf{i}}|0> . \tag{33}$$

Yet, the strong onsite correlations between the two species of charge carriers, necessary to introduce pairing in the Fermion subsystem in the first place, is counterproductive to such global superfluid phase correlations as the following identity shows

$$\prod_{\mathbf{i}} \frac{1}{\sqrt{2}}[\rho^+_{\mathbf{i}} + \tau^+_{\mathbf{i}}]|0> |0) = \frac{1}{2\pi}\int_{-\pi}^{+\pi} d\phi_{\mathbf{i}}[\cos(\phi_{\mathbf{i}})\tau^+_{\mathbf{i}} + \sin(\phi_{\mathbf{i}})][\sin(\phi_{\mathbf{i}})\rho^+_{\mathbf{i}} + \cos(\phi_{\mathbf{i}})]. \tag{34}$$

It in fact impies randomizing any potential off-diagonal order which would be necessary for establishing a global phase coherent state. The realization of a possible superfluid phase in such a scenario must be searched in a compromise between local and global phase correlations. Such competing behavior can be illustrated upon comparing the evolution of the onset temperatures T^* and T_ϕ controlling the correlators $< \rho^+_{\mathbf{i}}\tau^-_{\mathbf{i}} >$ and $< \rho^+_{\mathbf{q}=0}\rho^-_{\mathbf{q}=0} >$ as a function of g/t. This is shown in fig. 6 where one can clearly see the initial increase of the superconducting correlations together with the increase of local pair correlations as g/t increases. Beyond a certain critical value of g/t however, the superfluid correlations break down and the system collapses into an insulating states given by expression, eq. (32).

Let us now formulate this physics in terms of a functional integral representation of the Boson-Fermion model, which, after integrating out all single electron states, results in an effective action involving both, amplitude and phase fluctuations of the local an itinerant electron pairs[33]. This is done by introducing Grassmann variables $\{\bar{\Psi}_i, \Psi_i\}$ for the fermionic operators in a Nambu spinor representation and via a functional integral representation for the quantum spins representing the hard-core bosons of the localized electron-pairs on each lattice site. Those hardcore Bosons are parametrized by spherical coordinates describing a classical spin of magnitude $s = \frac{1}{2}$

$$\vec{\rho}_{\mathbf{i}} = s(\sin\theta_{\mathbf{i}}\cos\phi_{\mathbf{i}}, \sin\theta_{\mathbf{i}}\sin\phi_{\mathbf{i}}, \cos\theta_{\mathbf{i}}). \tag{35}$$

The correct quantification of the corresponding quantum pseudo-spin is assured by introducing a topological Wess-Zumino term in the effective action which has the form

$$A_{\rm WZ}[\bar{\Psi}_i, \Psi_i, \theta_i, \phi_i] = is\int d\tau \sum_i (1 - \cos\theta_i)\; \partial_\tau \phi_i. \tag{36}$$

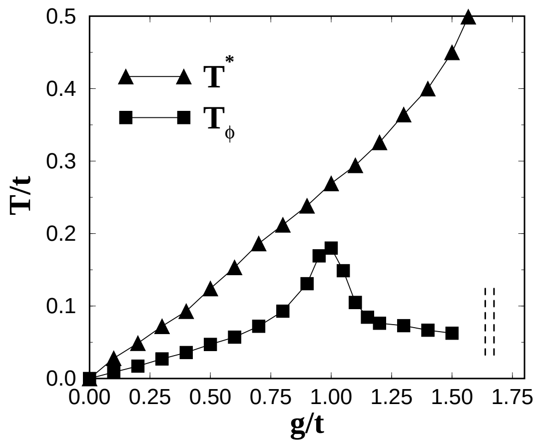

FIG. 6: Evolution of the onset temperatures T^* and T_ϕ of local and global phase correlations $<\rho^+_{\mathbf{i}}\tau^-_{\mathbf{i}}>$ and $<\rho^+_{\mathbf{q}=0}\rho^-_{\mathbf{q}=0}>$ as a function of the Boson-Fermion exchange coupling g (after an exact diagonalization study[34] on an 8-site ring).

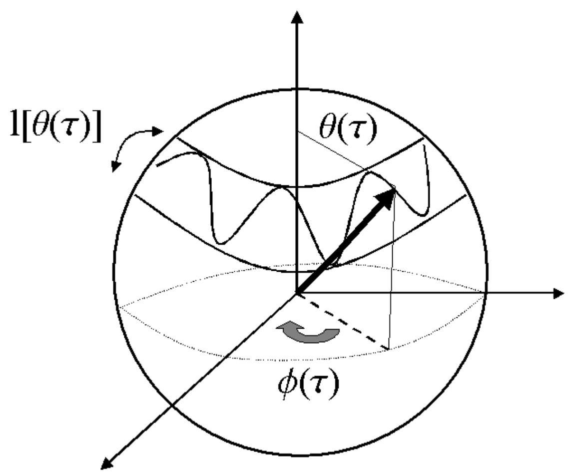

FIG. 7: Illustration of a typical path of the motion of the pseudospin on a given site precessing around the z-axis and following the evolution in time of the phase variable $\phi(\tau)$). $l[\theta(\tau)]$ indicates the amplitude of the pseudospin undulations driven by both, the fluctuations of the average boson density ($\langle\cos\theta\rangle$) and of the fluctuations of the pairing amplitude ($\langle\sin\theta\rangle$) (after ref.[33]).

The resulting effective action is a sum of terms involving the fluctuations of the phase $\phi_{\mathbf{i}}$ and the amplitude $sin\theta_{\mathbf{i}}$ of the pseudospin variable and the interaction involving the two

$$S = \int_0^\beta d\tau\,[S_\phi + S_\theta + S_{\phi-\theta}] \tag{37}$$

Assuming that the amplitude fluctuations are negligible (i.e., for paths of the pseudospin moving close to the equator of the sphere in fig. 7, which is the case for an density of local pairs around $n_B \simeq \frac{1}{2}$) we shall restrict the remaining discussion to a purely phase fluctuation driven superfluid state with a corresponding effective action given by

$$\begin{aligned} S_\phi &= -E_J \sum_{ij} \alpha_{ij} \cos[\phi_i(\tau) - \phi_j(\tau)] \\ &\quad + \sum_{ij} \frac{1}{8} \frac{\partial \phi_i(\tau)}{\partial \tau} C_{ij} \frac{\partial \phi_j(\tau)}{\partial \tau} + \sum_i \frac{i}{2} \frac{\partial \phi_i(\tau)}{\partial \tau} q_i(\tau) \end{aligned} \tag{38}$$

with $\alpha_{ij} = 1$ for i, j denoting nearest neighbor sites and being zero otherwise. What is immediately evident from the form of this effective phase-only part of this action of the Boson Fermion model is its similarity to that of Josephson junction arrays with the following correspondences:

- E_J controlling the tunneling of the bosons $\Longleftrightarrow$ Josephson coupling
- C_{ij} controlling the local and non-local density coupling $\Longleftrightarrow$ local and non-local capacitance
- q_i controlling the amplitude fluctuation induced local charge $\Longleftrightarrow$ offset charge.

In complete analogy to those widely studied Josephson junction array systems, this Boson-Fermion model scenario exhibits a Superconductor to Insulator transition. It is driven by a competition between the pair hopping-induced phase coherence and the *local charging effect* which is a function of the local boson density (or equivalently pairing-field amplitude) fluctuations. Nevertheless, noticeable differences of the action for the Boson-Fermion model and that of the Josephson-junction array systems exist:
(i) the effective coupling constants now depend in a highly non-trivial manner on the original parameters of the underlying Boson-Fermion model hamiltonian which gives rise, as we shall see below, to an intricate dependence of the phase diagram on the two parameters, g/t and the boson concentration n_B.
(ii) the offset charge $q_i = \mu/g + 1 - cos\theta \equiv \mu/g + 1 - n_B$ is controlled by the topological Wess Zumino term, leading to a time dependence of this offset charge caused by a coupling between the phase and the concentration (or alterantively the amplitude) fluctuations of the local pairs. As a consequence the physics of this Boson-Fermion model is controlled not only by the parameters g/t and $n_{\rm tot} = n_F + n_B$ but also by the ratio n_F/n_B[33]. Thus, for fixed values of g/t and a total density $n_{\rm tot}$ the parameter which controls both E_J and C_{ij} is given by $\tilde{g} = 2g\sqrt{n_B(n_B-1)}$. Hence, as n_B approaches either the very dilute or very dense limit $n_B = 0, 1$, the expected superfluid transition temperature goes to zero, given the assumption that the amplitude fluctuations in that case play a minor role. On the other hand, by suitably monitoring the total local charge one can obtain a stable superfluid state. To extract this type of physics one has to resort to a coarse-graining description[35] with $< e^{i\phi_i} >$ taken as an order parameter. The derivation of that is standard but rather involved and we refer the reader to refs.[33,35] for details. Such a procedure leads to an effective free energy given by

$$F_\psi = \int_0^\beta d\tau d\tau^{'} \sum_{ij} \psi_i^*(\tau) \left[\alpha_{ij}\delta(\tau-\tau^{'}) - \chi_{ij}(\tau,\tau^{'})\right] \psi_j(\tau^{'}), \tag{39}$$

with

$$\chi_{ij}(\tau,\tau^{'}) = \langle e^{i\left[\phi_i(\tau)-\phi_j(\tau)^{'}\right]}\rangle_0 \tag{40}$$

and where $\psi_i^*(\tau)$ are auxiliary Hubbard-Stratonovic fields conjugated to $< e^{i\phi_{\rm i}} >$. The explicit evaluation of the phase correlator[36] permits to reformulate the effective action, eq. (38), in terms of a Ginzburg Landau free energy functional in momentum-frequency representation:

$$F_\psi = \frac{1}{\beta L}\sum_{n,k} \psi_k^*(\omega_n)\left[\alpha_k^{-1} - \chi_k(\omega_n)\right]\psi_k(\omega_n)\,. \tag{41}$$

An expansion in terms of small momentum vectors k and Matsubara frequencies ω_n yields

$$F_\psi = \frac{1}{\beta L}\sum_{k,n}\left[\frac{2}{zE_J} - \chi_0 + ak^2 + b\omega_n^2 + i\lambda\omega_n + ...\right]|\psi_k(\omega_n)|^2 \tag{42}$$

where b, and λ are the coefficients of the expansion of $\chi_k(\omega_n)$ around the limit $\omega_n = 0$.

The superfluid phase separation line is then determined by the conditions that the coefficient of the quadratic terms in k and ω_n vanish, i.e.,

$$1 - \frac{zE_J}{2}\chi_0(0) = 0\,. \tag{43}$$

The phase diagram which results from this is illustrated in fig. 8. It tracks the gross features of the abrupt beakdown of the superfluid phase with increasing g/t as already forshadowed in a study based on small clusters[34] which shows the building up and subsequent breaking down of the phase correlations, fig. 6. These findings clearly suggest that strong coupling electron-lattice systems in the cross-over regime of adiabaticity can truely give rise not only to a superfluid phase but also to an insulating Bipolaron state. We stress however that such an insulating state of Bipolarons would be the result of a non-translational symmetry breaking cooperative phenomenon, similar to that of the Mott transition in correlated systems. It thus differs significantly from an insulating state of disordered non-overlapping localized Bipolarons on a lattice such as could be conjectured on the basis of a semi-classical approach and presented in section III in my introductory lecture: “Introduction to polaron physics: concepts and model”.

V. CONCLUSION

Studies devoted to the cross-over from the weak to strong coupling regime and from the adiabatic to the non-adiabatic limit generally involves the concept of lattice polarons, such as formulated in the paradigme of the well studied Holstein model. This model here plays the same role as the Hubbard model for systems with strong electron correlations. Here as well as there, studying real materials can bring in new and hiherto perhaps unsuspected features which might turn out to be of considerable relevance. In the treatise developed in this lecture I have been guided by the well established theoretical results of the abrupt change-over from itinerant to almost localized polaronic states (so well documented in the various theoretical lectures presented here) and conjectured that this scenario would hold in a dense polaronic system. To within a first approximation we can describe such physics in terms of an effective model—the Boson-Fermion model—involving itinerant non-interacting electrons on an undeformable lattice and localized Bipolarons with an exchange coupling between the two. Such a picture contains only two relevant parameters: the ratio of the exchange coupling to the electron hopping integral and the relative density of charge carriers of the two species; the adiabiticity ratio being taken of the order unity. Sofar it has not been possible to derive this effective Boson-Fermion model scenario from the Holstein Hamiltonian. Yet, it permits to relatively easyly obtain results on the spectral properties of the electrons, the phonons, local dynamical lattice deformations etc., which can be tested on real materials and which in fact can and have confirmed such theoretical predictions. It might well turn out in the near future that studies of real materials which show cross-over features will require some perhaps substantial revisions of the Holstein model in the sense that local Martensitic like lattice instabilities have to be incorporated in form of some local polaron physics and which would involve the interplay of the metal ions and their ligand environements. Such studies are presently being undertaken, but a discussion of that is too untimely and should be defered to some later date.

One of the key points I wanted to promulgate in this lecture was the possibility of a Superconductor to Bipolaronic Insulator phase transition for polaronic systems in the strong coupling regime and in the cross-over between adiabatic and anti-adiabatic behavior ($\omega_0/t \simeq 1$) which is believed to be describable within the Boson-Fermion model scenario. The superfluid phase which results in such a situation contains features which are common to those encountered in classical BCS superconductors (showing the opening of a gap in the single particle electron spectrum) and in supefluid systems with collective phase oscillations (showing soundwave like excitations in the Cooperon channel)[?] . We found as an alternative to such a superfluid phase an insulating phase, reminiscent of a Mott insulator caused by the predominance of local correlations between the Bipolarons and itinerant electron pairs over their long range phase correlations between them. This Bipolaron Insulator is quite different from a conceivable state of localized Bipolarons randomly distributed on a lattice and which would come about by argumenting on the basis of a semi-classical discription of the polaron problem, such as presented in my Introductrory course to polaron physics ("Introduction to polaron physics: Basic concepts and Models") in this volume (see in particular the discussion around Fig. 1 in section III of this contribution). The insulating state discussed here results from a collective phenomenon.

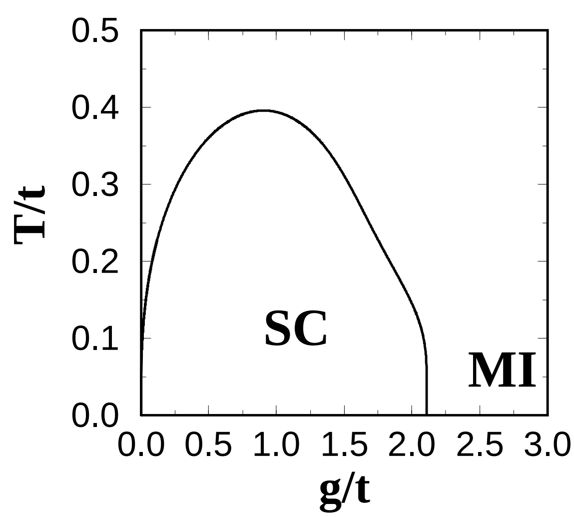

FIG. 8: Phasediagram of the BFM showing as a function of g/t the boundary between a Mott insulating (MI) state with homogeneous charge distribution and a superconducting (SC) phase with long range phase coherence in the representative case of $\Delta_B = 0, n_{F\uparrow} = n_{F\downarrow} = 2n_B = 1$) (after ref.[33]).

VI. ACKNOWLEDGEMENTS

This lecture is dedicated to B. K. Chakraverty. Following my critizisms of his proposed Bipolaronic Insulator phase[9], his incessant attacks on the competing idea of a Bipolaronic Superconductor phase[10] motivated me to propose the scenario of resonating Bipolarons and the Boson-Fermion model in the early eighties and which was subsequently studied in detail over the past twenty years in Grenoble. I acknowledge the active participation of my collaborators on that, and particularly: M. Cuoco, T. Domanski, E. de Mello, T. Kostyrko, M. Robin and A. Romano.

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